L-Valine, N-(3,4-difluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C21H31F2NO3/c1-4-5-6-7-8-9-10-13-27-21(26)19(15(2)3)24-20(25)16-11-12-1
InchiKey: NMLIITUQKDBZTP-UHFFFAOYSA-N
Formula: C21H31F2NO3
SMILES: CCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C
Mol. weight [g/mol]: 383.47

Physical Properties

Property code	Value	Unit	Source
gf	-448.86	kJ/mol	Joback Method
hf	-969.87	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.013		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	894.51	K	Joback Method
tc	1097.76	K	Joback Method
tf	523.82	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.37	J/mol×K	894.51	Joback Method
cpg	997.83	J/mol×K	928.38	Joback Method
cpg	1012.15	J/mol×K	962.26	Joback Method
cpg	1025.34	J/mol×K	996.13	Joback Method
cpg	1037.46	J/mol×K	1030.01	Joback Method
cpg	1048.53	J/mol×K	1063.88	Joback Method
cpg	1058.60	J/mol×K	1097.76	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume